

Quantum decoration transformation for spin models

F. F. Braz, F. C. Rodrigues, S. M. de Souza and Onofre Rojas¹

Departamento de Física, Universidade Federal de Lavras, CP 3037, 37200-000, Lavras-MG, Brazil

Abstract

It is quite relevant the extension of decoration transformation for quantum spin models since most of the real materials could be well described by Heisenberg type models. Here we propose an exact quantum decoration transformation and also showing interesting properties such as the persistence of symmetry and the symmetry breaking during this transformation. Although the proposed transformation, in principle, cannot be used to map exactly a quantum spin lattice model into another quantum spin lattice model, since the operators are non-commutative. However, it is possible the mapping in the "classical" limit, establishing an equivalence between both quantum spin lattice models. To study the validity of this approach for quantum spin lattice model, we use the Zassenhaus formula, and we verify how the correction could influence the decoration transformation. But this correction could be useless to improve the quantum decoration transformation because it involves the second-nearest-neighbor and further nearest neighbor couplings, which leads into a cumbersome task to establish the equivalence between both lattice models. This correction also gives us valuable information about its contribution, for most of the Heisenberg type models, this correction could be irrelevant at least up to the third order term of Zassenhaus formula. This transformation is applied to a finite size Heisenberg chain, comparing with the exact numerical results, our result is consistent for weak xy-anisotropy coupling. We also apply to bond-alternating Ising-Heisenberg chain model, obtaining an accurate result in the limit of the quasi-Ising chain.

1. Introduction

A considerable number of classical decorated Ising models have been solved using the decoration transformation proposed in the 1950s by M. E. Fisher[1] and Syozi[2], since that, this transformation was useful to study decorated Ising lattice in triangular, honeycomb, Kagomé, and bathroom-tile lattices[3, 4, 5, 6], as well as the Union Jack (centered square)[7] and the square Kagomé[8] lattice, later pentagonal lattice also was considered by Urumov[9] and by Rojas et al.[10] among others. Motivated by the above results, later this approach was generalized in reference [11] for arbitrary spin, such as the classical-quantum spin models. The decoration transformation can also be applied to classical-quantum spin models, such as Ising-Heisenberg models. Several quasi-one-dimensional models have been investigated, similar to that diamond-like chain[12, 13, 14, 15, 16, 17, 18, 19, 20] and references therein, as well as two-dimensional lattice spin models [21, 22, 23, 24, 25, 26, 27, 28, 29]. Furthermore, it can be applied even for three-dimensional decorated systems[30], this approach can also be applied combining with Monte Carlo simulation for 3D systems[31, 32].

Classical decoration transformation could be applied beyond spin models, such as localized Ising spins and itinerant electrons in two-dimensional models as discussed by Strecka et al.[23]. Later, the decoration transformation approach has also been applied to spinless interacting particles, which shows the possibility of application for interacting electron models[33]. Due to these meaningful signs of progress, Strecka[34] discussed this transformation in a more detailed fashion, following the approach proposed in reference [11] for the case of quantum-classical models. Recently, another interesting transformation[35] was also suggested to avoid applying several steps of decoration transformations, by using just one transformation. Alternatively, Derzhko et al.[40] proposed a perturbative approach to study the almost Ising-Heisenberg diamond chain, by adding a small contribution in XY part.

It is of great importance the extension of classical decoration transformation for the quantum spin models, because most of the real materials could be well described by Heisenberg type models. Besides, recent investigations concerning thermal entanglement have motivated also this mapping such as q-bits bonded by Heisenberg coupling with finite number of sites. Thus, quantum decoration transformation could be potentially applied for small quantum systems in [36, 37, 38, 39] and references therein.

^{*}email: ors@dfi.uflla.br

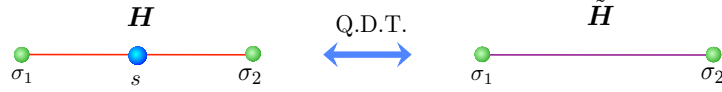


Figure 1: Schematic representation of quantum decoration transformation. Where s corresponds to decorated spin, while σ_1 and σ_2 correspond to Heisenberg spins, H (\tilde{H}) corresponds to decorated (effective) Hamiltonian respectively.

In this paper, we present a pure quantum decoration transformation for a quantum mixed or decorated quantum spin model into an effective quantum spin model. The main difference between the classical and quantum transformation is the non-commutative property; consequently, the Boltzmann factor becomes an operator. A basic idea of quantum decoration transformation already has been discussed for a particular case of diluted Heisenberg model [41]. To introduce a quantum version of decoration transformation for Heisenberg spin models into an uniform spin-1/2 Heisenberg model, we will follow the basic idea used by Dunn and Essam[41], as well as by M. E. Fisher [1] and Syozi[2].

This paper is organized as follows, in sec. 2 we present the two-leg quantum decoration transformation, where is included a couple of applications. In sec. 3 we show the star-triangle decoration transformation, we also give a couple of applications for the star-triangle transformation. Whereas, in sec. 4 we discuss how to apply for a quantum spin lattice model, the correction of the transformation can be obtained using the Zassenhaus formula. Besides, we apply for finite size Heisenberg model as well as for bond alternating Ising-Heisenberg model. Finally, in sec. 5 we give our conclusion and perspectives.

2. Two leg-star quantum decoration transformation

To proceed with decoration transformation, we need to extend the Boltzmann factor[1, 2, 11] to some operator, which can bring all information about the quantum decorated Hamiltonian.

Therefore, let us consider a decorated system illustrated in fig.1, composed of arbitrary quantum operators σ_1 , σ_2 , and s is any other quantum operator or operators called “decorated operator”. Defining the operator \mathbf{W} as $\mathbf{W} = e^{-\beta \mathbf{H}}$, where \mathbf{H} is the Hamiltonian of decorated system illustrated on left side of fig.1, and $\beta = \frac{1}{k_B T}$, with k_B being the Boltzmann constant and T is the absolute temperature.

Assuming the Hamiltonian \mathbf{H} 's eigenvalues as ε_n , and denoting the corresponding orthonormal eigenvectors by $|\eta_n\rangle$. Thus, the operator \mathbf{W} can be expressed by

$$\mathbf{W} = e^{-\beta \mathbf{H}} = \sum_{n=1}^{\dim(H)} e^{-\beta \varepsilon_n} |\eta_n\rangle \langle \eta_n|, \quad (1)$$

where $\dim(H)$ means the dimension of the Hamiltonian \mathbf{H} .

Multiplying both sides of operator \mathbf{W} by the identity operator $\mathbf{1} = \sum_{s, \sigma_1, \sigma_2} |s, \sigma_1, \sigma_2\rangle \langle s, \sigma_1, \sigma_2|$, we have

$$\begin{aligned} \mathbf{W} &= \sum_{s, \sigma_1, \sigma_2} \sum_{s', \sigma'_1, \sigma'_2} |s, \sigma_1, \sigma_2\rangle \langle s, \sigma_1, \sigma_2| e^{-\beta \mathbf{H}} |s', \sigma'_1, \sigma'_2\rangle \langle s', \sigma'_1, \sigma'_2|, \\ &= \sum_{s, \sigma_1, \sigma_2} \sum_{s', \sigma'_1, \sigma'_2} \langle s, \sigma_1, \sigma_2| e^{-\beta \mathbf{H}} |s', \sigma'_1, \sigma'_2\rangle |s, \sigma_1, \sigma_2\rangle \langle s', \sigma'_1, \sigma'_2|, \\ &= \sum_{n=1}^{\dim(H)} \sum_{s, \sigma_1, \sigma_2} \sum_{s', \sigma'_1, \sigma'_2} e^{-\beta \varepsilon_n} \langle s, \sigma_1, \sigma_2| \eta_n\rangle \langle \eta_n| s', \sigma'_1, \sigma'_2\rangle |s, \sigma_1, \sigma_2\rangle \langle s', \sigma'_1, \sigma'_2|, \\ &= \sum_{n=1}^{\dim(H)} \sum_{s, \sigma_1, \sigma_2} \sum_{s', \sigma'_1, \sigma'_2} e^{-\beta \varepsilon_n} c_{s, \sigma_1, \sigma_2}^{n*} c_{s', \sigma'_1, \sigma'_2}^n |s, \sigma_1, \sigma_2\rangle \langle s', \sigma'_1, \sigma'_2|, \end{aligned} \quad (2)$$

where the coefficients are denoted by $c_{s, \sigma_1, \sigma_2}^n = \langle \eta_n | s, \sigma_1, \sigma_2 \rangle$ and $c_{s, \sigma_1, \sigma_2}^{n*} = \langle s, \sigma_1, \sigma_2 | \eta_n \rangle$.

Now, let us calculate the partial trace over decorated quantum operator s , this result is still an operator, called the reduced operator \mathbf{W}_r , which is expressed as

$$\mathbf{W}_r = \text{tr}_s (e^{-\beta \mathbf{H}}) = \sum_s \langle s | \mathbf{W} | s \rangle. \quad (4)$$

Explicitly, the partial trace in decorated quantum operator becomes

$$\mathbf{W}_r = \sum_{n=1}^{\dim(H)} \sum_{s, \sigma_1, \sigma_2} \sum_{\sigma'_1, \sigma'_2} e^{-\beta \varepsilon_n} c_{s, \sigma_1, \sigma_2}^{n*} c_{s, \sigma'_1, \sigma'_2}^n |\sigma_1, \sigma_2\rangle \langle \sigma'_1, \sigma'_2|, \quad (5)$$

where we assume the following partial scalar product in \mathbf{s} : $|\sigma_1, \sigma_2\rangle = \langle s | s, \sigma_1, \sigma_2 \rangle$ and $\langle \sigma_1, \sigma_2 | = \langle s, \sigma_1, \sigma_2 | s \rangle$. Using this result, we can rewrite the elements of reduced operator \mathbf{W}_r simply as

$$r_{\sigma_1, \sigma_2; \sigma'_1, \sigma'_2} = \sum_{n=1}^{\dim(H)} \sum_s e^{-\beta \varepsilon_n} c_{s, \sigma_1, \sigma_2}^{n*} c_{s, \sigma'_1, \sigma'_2}^n. \quad (6)$$

On the other hand, the transformed system is schematically represented on the right side of fig.1. Note that the reduced operator \mathbf{W}_r only depends on quantum operators σ_1 and σ_2 . Therefore, we define another operator $\tilde{\mathbf{W}} = e^{-\beta \tilde{\mathbf{H}}}$, with $\tilde{\mathbf{H}}$ being the Hamiltonian of the transformed system or simply called the effective Hamiltonian.

Therefore, multiplying both sides of operator $\tilde{\mathbf{W}}$ by the identity operator $\mathbf{1} = \sum_{\sigma_1, \sigma_2} |\sigma_1, \sigma_2\rangle \langle \sigma_1, \sigma_2|$, we have

$$\begin{aligned} \tilde{\mathbf{W}} &= \sum_{\sigma_1, \sigma_2} \sum_{\sigma'_1, \sigma'_2} |\sigma_1, \sigma_2\rangle \langle \sigma_1, \sigma_2| e^{-\beta \tilde{\mathbf{H}}} |\sigma'_1, \sigma'_2\rangle \langle \sigma'_1, \sigma'_2|, \\ &= \sum_{n=1}^{\dim(\tilde{H})} \sum_{\sigma_1, \sigma_2} \sum_{\sigma'_1, \sigma'_2} e^{-\beta \tilde{\varepsilon}_n} \tilde{c}_{\sigma_1, \sigma_2}^{n*} \tilde{c}_{\sigma'_1, \sigma'_2}^n |\sigma_1, \sigma_2\rangle \langle \sigma'_1, \sigma'_2|, \end{aligned} \quad (7)$$

where $\tilde{c}_{\sigma_1, \sigma_2}^n = \langle \zeta_n | \sigma_1, \sigma_2 \rangle$ and $\tilde{c}_{\sigma_1, \sigma_2}^{n*} = \langle \sigma_1, \sigma_2 | \zeta_n \rangle$. Similarly, we are considering $\tilde{\varepsilon}_n$ and $|\zeta_n\rangle$ being the eigenvalues and eigenvectors of the effective Hamiltonian $\tilde{\mathbf{H}}$.

Furthermore, the elements of $\tilde{\mathbf{W}}$ are given by

$$\tilde{r}_{\sigma_1, \sigma_2; \sigma'_1, \sigma'_2} = \sum_{n=1}^{\dim(\tilde{H})} e^{-\beta \tilde{\varepsilon}_n} \tilde{c}_{\sigma_1, \sigma_2}^{n*} \tilde{c}_{\sigma'_1, \sigma'_2}^n. \quad (8)$$

Imposing the condition of \mathbf{W}_r and $\tilde{\mathbf{W}}$ must be identical, where both of them depend only of σ_1 and σ_2 operators. Consequently, all elements of \mathbf{W}_r and $\tilde{\mathbf{W}}$ are related by

$$r_{\sigma_1, \sigma_2; \sigma'_1, \sigma'_2} = \tilde{r}_{\sigma_1, \sigma_2; \sigma'_1, \sigma'_2}. \quad (9)$$

Surely, this is a natural generalization of classical decoration transformation, considered initially in reference [1, 2, 11].

Notice that, performing the trace over all spins of decorated system, one must obtain the partition function of the system $Z = \text{tr}(\mathbf{W})$, with tr denoting the total trace. The operator \mathbf{W} divided by Z will be nothing else than the density operator of the system $\rho = \frac{\mathbf{W}}{Z}$.

The above transformation could be applied for a series of Heisenberg spin models, in this sense, we consider some particular cases to illustrate this transformation.

2.1. Quantum decoration transformation for spin- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ model

First, let us consider a simple system composed only of three spins, as represented schematically by fig.1, with Heisenberg coupling, then, the Hamiltonian of decorated spin- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ model can be written as

$$\mathbf{H} = -J[s^x(\sigma_1^x + \sigma_2^x) + s^y(\sigma_1^y + \sigma_2^y)] - \Delta s^z(\sigma_1^z + \sigma_2^z) - h(\sigma_1^z + \sigma_2^z) - h_1 s^z, \quad (10)$$

where $\sigma_i^x = \frac{1}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_i^y = \frac{1}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ and $\sigma_i^z = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ are spin-1/2 operators, with $i = \{1, 2\}$, and the decorated operator s^α (with $\alpha = \{x, y, z\}$) are also another spin-1/2 operators, same as defined for σ_i^α operators. Whereas, J is the exchange interaction parameter in xy axes, and Δ is the anisotropic exchange interaction in z axis. Here $h = gB$ and $h_1 = g_1 B$, with B being the magnetic field acting in σ_1^z , σ_2^z and s^z , while g_1 (g) is the Landé g-factor for s^z (σ_1^z and σ_2^z), respectively.

To diagonalize the Hamiltonian \mathbf{H} , we express the Hamiltonian in the natural basis $\{|\sigma_1, \sigma_2\rangle\} = \{|\uparrow, +, +\rangle, |\uparrow, +, -\rangle, |\uparrow, -, +\rangle, |\uparrow, -, -\rangle, |\downarrow, +, +\rangle, |\downarrow, +, -\rangle, |\downarrow, -, +\rangle, |\downarrow, -, -\rangle\}$, for details see Appendix (A.1).

Hereafter the diagonalization of the Hamiltonian (10) is performed, the eigenvalues of the Hamiltonian \mathbf{H} are given by

$$\begin{aligned}\varepsilon_1 &= -\frac{\Delta}{2} - \frac{h_1}{2} - h, & \varepsilon_2 &= -\frac{h_1}{2}, & \varepsilon_3 &= \frac{\Delta}{4} - \frac{h}{2} + \frac{\theta}{4}, & \varepsilon_4 &= \frac{\Delta}{4} - \frac{h}{2} - \frac{\theta}{4}, \\ \varepsilon_5 &= \frac{h_1}{2}, & \varepsilon_6 &= \frac{\Delta}{4} + \frac{h}{2} + \frac{\vartheta}{4}, & \varepsilon_7 &= \frac{\Delta}{4} + \frac{h}{2} - \frac{\vartheta}{4}, & \varepsilon_8 &= -\frac{\Delta}{2} + \frac{h_1}{2} + h,\end{aligned}\quad (11)$$

with $\theta = \sqrt{(\Delta + 2h - 2h_1)^2 + 8J^2}$ and $\vartheta = \sqrt{(\Delta - 2h + 2h_1)^2 + 8J^2}$.

Whereas, the corresponding eigenvectors are given respectively by

$$\begin{aligned}|\eta_1\rangle &= |\uparrow, +, +\rangle, \\ |\eta_2\rangle &= \frac{1}{\sqrt{2}}(|\uparrow, +, -\rangle - |\uparrow, -, +\rangle), \\ |\eta_3\rangle &= \frac{1}{\sqrt{2}}\sin(\phi)|\uparrow, +, -\rangle + \frac{1}{\sqrt{2}}\sin(\phi)|\uparrow, -, +\rangle + \cos(\phi)|\downarrow, +, +\rangle, \\ |\eta_4\rangle &= \frac{1}{\sqrt{2}}\cos(\phi)|\uparrow, +, -\rangle + \frac{1}{\sqrt{2}}\cos(\phi)|\uparrow, -, +\rangle - \sin(\phi)|\downarrow, +, +\rangle, \\ |\eta_5\rangle &= \frac{1}{\sqrt{2}}(|\downarrow, +, -\rangle - |\downarrow, -, +\rangle), \\ |\eta_6\rangle &= \frac{1}{\sqrt{2}}\sin(\varphi)|\downarrow, +, -\rangle + \frac{1}{\sqrt{2}}\sin(\varphi)|\downarrow, -, +\rangle - \cos(\varphi)|\uparrow, -, -\rangle, \\ |\eta_7\rangle &= \frac{1}{\sqrt{2}}\cos(\varphi)|\downarrow, +, -\rangle + \frac{1}{\sqrt{2}}\cos(\varphi)|\downarrow, -, +\rangle + \sin(\varphi)|\uparrow, -, -\rangle, \\ |\eta_8\rangle &= |\downarrow, -, -\rangle,\end{aligned}\quad (12)$$

with

$$\phi = \tan^{-1}\left(\frac{\theta - (\Delta + 2h - 2h_1)}{2\sqrt{2}J}\right), \quad \text{and} \quad -\frac{\pi}{2} \leq \phi \leq \frac{\pi}{2}, \quad (13)$$

$$\varphi = \tan^{-1}\left(\frac{\vartheta - (\Delta - 2h + 2h_1)}{2\sqrt{2}J}\right), \quad \text{and} \quad -\frac{\pi}{2} \leq \varphi \leq \frac{\pi}{2}. \quad (14)$$

Furthermore, performing the partial trace in s using eq.(4), we obtain the reduced operator \mathbf{W}_r in terms of natural basis $\{|\sigma_1, \sigma_2\rangle\} = \{|\uparrow, +\rangle, |\uparrow, -\rangle, |\downarrow, +\rangle, |\downarrow, -\rangle\}$. Thus, the operator becomes

$$\mathbf{W}_r = \begin{bmatrix} w_1 & 0 & 0 & 0 \\ 0 & \frac{w_2 + w_3}{2} & \frac{w_2 - w_3}{2} & 0 \\ 0 & \frac{w_2 - w_3}{2} & \frac{w_2 + w_3}{2} & 0 \\ 0 & 0 & 0 & w_4 \end{bmatrix}, \quad (15)$$

where the elements of \mathbf{W}_r are obtained from eq.(6), and result in

$$w_1 = r_{1,1} = \sum_{n=1}^{\dim(\tilde{H})} \sum_{s=\uparrow, \downarrow} e^{-\beta\varepsilon_n} |c_{s,+,+}^n|^2, \quad (16)$$

$$\frac{w_2 + w_3}{2} = r_{2,2} = \sum_{n=1}^{\dim(\tilde{H})} \sum_{s=\uparrow, \downarrow} e^{-\beta\varepsilon_n} |c_{s,+,-}^n|^2, \quad (17)$$

$$\frac{w_2 - w_3}{2} = r_{2,3} = \sum_{n=1}^{\dim(\tilde{H})} \sum_{s=\uparrow, \downarrow} e^{-\beta\varepsilon_n} c_{s,+, -}^{n*} c_{s, -, +}^n, \quad (18)$$

$$w_4 = r_{4,4} = \sum_{n=1}^{\dim(\tilde{H})} \sum_{s=\uparrow, \downarrow} e^{-\beta\varepsilon_n} |c_{s,-,-}^n|^2. \quad (19)$$

After using some algebraic manipulation, we express the elements of \mathbf{W}_r in natural basis, as a function of w_1, \dots, w_4 , which are given explicitly as

$$w_1 = e^{-\frac{\beta(\Delta - 2h + \theta)}{4}} \cos^2(\phi) + e^{-\frac{\beta(\Delta - 2h - \theta)}{4}} \sin^2(\phi) + e^{\frac{\beta(\Delta + h_1 + 2h)}{2}}, \quad (20)$$

$$w_2 = \left(e^{\frac{\beta\theta}{4}} \cos^2(\phi) + e^{-\frac{\beta\theta}{4}} \sin^2(\phi)\right) e^{-\frac{\beta(\Delta - 2h)}{4}} + \left(e^{-\frac{\beta\vartheta}{4}} \sin^2(\varphi) + e^{\frac{\beta\vartheta}{4}} \cos^2(\phi)\right) e^{-\frac{\beta(\Delta + 2h)}{4}}, \quad (21)$$

$$w_3 = 2 \cosh\left(\frac{\beta h_1}{2}\right), \quad (22)$$

$$w_4 = e^{-\frac{\beta(\Delta + 2h + \vartheta)}{4}} \cos^2(\varphi) + e^{-\frac{\beta(\Delta + 2h - \vartheta)}{4}} \sin^2(\varphi) + e^{\frac{\beta(\Delta - h_1 - 2h)}{2}}. \quad (23)$$

Alternatively, one can express \mathbf{W}_r as a function of orthogonal projection operators (eigenvectors basis)

$$\mathbf{W}_r = \sum_{k=1}^4 w_k |\varsigma_k\rangle \langle \varsigma_k|, \quad (24)$$

where

$$|\varsigma_1\rangle = |++\rangle, \quad |\varsigma_2\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle), \quad |\varsigma_3\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \quad \text{and} \quad |\varsigma_4\rangle = |--\rangle. \quad (25)$$

A similar notation was also used in reference [41], for diluted Heisenberg model.

On the other hand, let us consider the effective Hamiltonian of spin- $(\frac{1}{2}, \frac{1}{2})$ XXZ model as

$$\tilde{H} = -\tilde{J}_0 - \tilde{J}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) - \tilde{\Delta} \sigma_1^z \sigma_2^z - \tilde{h}(\sigma_1^z + \sigma_2^z), \quad (26)$$

where \tilde{J}_0 is a “constant” energy, \tilde{J} is the effective exchange parameter between σ_1 and σ_2 in xy axes, $\tilde{\Delta}$ represents the effective exchange parameter in z axis. Whereas $\tilde{h} = g\tilde{B}$, \tilde{B} represents the effective external magnetic field in both operators σ_1^z and σ_2^z , with g being the Landé g-factor.

Writing in the natural basis $\{|\sigma_1, \sigma_2\rangle\}$, the Hamiltonian \tilde{H} becomes

$$\tilde{H} = \begin{bmatrix} -\tilde{J}_0 - \frac{\tilde{\Delta}}{4} - \tilde{h} & 0 & 0 & 0 \\ 0 & -\tilde{J}_0 + \frac{\tilde{\Delta}}{4} & -\frac{\tilde{J}}{2} & 0 \\ 0 & -\frac{\tilde{J}}{2} & -\tilde{J}_0 + \frac{\tilde{\Delta}}{4} & 0 \\ 0 & 0 & 0 & -\tilde{J}_0 - \frac{\tilde{\Delta}}{4} + \tilde{h} \end{bmatrix}. \quad (27)$$

Using the Hamiltonian (27), we can define the operator $\tilde{W} = e^{-\beta \tilde{H}}$, in a standard basis $\{|\sigma_1, \sigma_2\rangle\}$. Hence, \tilde{W} matrix is given explicitly by

$$\tilde{W} = \begin{bmatrix} \tilde{w}_1 & 0 & 0 & 0 \\ 0 & \frac{\tilde{w}_2 + \tilde{w}_3}{2} & \frac{\tilde{w}_2 - \tilde{w}_3}{2} & 0 \\ 0 & \frac{\tilde{w}_2 - \tilde{w}_3}{2} & \frac{\tilde{w}_2 + \tilde{w}_3}{2} & 0 \\ 0 & 0 & 0 & \tilde{w}_4 \end{bmatrix}, \quad (28)$$

where the elements of \tilde{W} can be expressed regarding the effective Hamiltonian parameters

$$\tilde{w}_1 = e^{-\beta(-\tilde{J}_0 - \frac{\tilde{\Delta}}{4} - \tilde{h})}, \quad \tilde{w}_2 = e^{-\beta(-\tilde{J}_0 + \frac{\tilde{\Delta}}{4} - \frac{\tilde{J}}{2})}, \quad \tilde{w}_3 = e^{-\beta(-\tilde{J}_0 + \frac{\tilde{\Delta}}{4} + \frac{\tilde{J}}{2})} \quad \text{and} \quad \tilde{w}_4 = e^{-\beta(-\tilde{J}_0 - \frac{\tilde{\Delta}}{4} + \tilde{h})}. \quad (29)$$

Equivalently, using the projection operator, analogous to operator eq.(24), we also have

$$\tilde{W} = \sum_{k=1}^4 \tilde{w}_k |\varsigma_k\rangle \langle \varsigma_k|, \quad (30)$$

where $|\varsigma_k\rangle$ are the eigenvectors of \tilde{W} , the same obtained in (25), and obviously satisfy $[\mathbf{W}_r, \tilde{W}] = 0$.

Now, we can impose that the corresponding element must be identical for both operators and assuming $\tilde{w}_1 = w_1$, $\tilde{w}_2 = w_2$, $\tilde{w}_3 = w_3$ and $\tilde{w}_4 = w_4$. Besides, this condition establishes a system of algebraic equation, with 4 unknown parameters \tilde{J}_0 , \tilde{J} , $\tilde{\Delta}$ and \tilde{h} , which can be obtained as a function of decorated Hamiltonian parameters J , Δ , h and h_1 . For instance, let us write just as a function of w_1 , w_2 , w_3 and w_4 , which are explicitly determined by eqs.(20-23). Thus, solving the algebraic system, we have

$$\tilde{J}_0 = \frac{1}{4\beta} \ln(w_1 w_2 w_3 w_4), \quad \tilde{\Delta} = \frac{1}{\beta} \ln\left(\frac{w_1 w_4}{w_2 w_3}\right), \quad \tilde{h} = \frac{1}{2\beta} \ln\left(\frac{w_1}{w_4}\right) \quad \text{and} \quad \tilde{J} = \frac{1}{\beta} \ln\left(\frac{w_2}{w_3}\right). \quad (31)$$

Finally, one can see the results for \tilde{J}_0 , $\tilde{\Delta}$ and \tilde{h} in terms of w_1 , w_2 , w_3 and w_4 are quite similar to the classical decoration transformation[1, 2, 11]. Whereas the quantum parameter \tilde{J} vanishes when $w_2 = w_3$ following the eq.(31), because $J = 0$ in the original Hamiltonian.

2.2. Quantum decoration transformation for spin-(1, $\frac{1}{2}$, $\frac{1}{2}$) XXZ model

In what follows, we consider a system composed by three spins, one quantum decorated spin-1 and two quantum spin-1/2. Thus, the Hamiltonian of decorated spin-(1, $\frac{1}{2}$, $\frac{1}{2}$) XXZ model, is given by

$$\mathbf{H} = -J[s^x(\sigma_1^x + \sigma_2^x) + s^y(\sigma_1^y + \sigma_2^y)] - \Delta s^z(\sigma_1^z + \sigma_2^z). \quad (32)$$

The definition of the model is quite similar to the previous one; the only difference is s^α now becomes $s^x = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$, $s^y = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}$, $s^z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$. Whereas σ_1^α and σ_2^α , (with $\alpha = \{x, y, z\}$) are spin-1/2 operators as defined in previous section. The Hamiltonian in natural basis $\{|s, \sigma_1, \sigma_2\rangle\}$, becomes a 12×12 matrix. The representation of the matrix \mathbf{H} is shown in the Appendix eq.(A.2).

After diagonalizing the Hamiltonian (32), we obtain the following eigenvalues

$$\begin{aligned} \varepsilon_1 = \varepsilon_{12} = -\Delta, \quad \varepsilon_2 = \varepsilon_9 = J, \quad \varepsilon_3 = \varepsilon_{10} = -J, \\ \varepsilon_4 = \varepsilon_8 = \varepsilon_{11} = 0, \quad \varepsilon_5 = \frac{\Delta}{2} + \frac{\Delta}{2\cos(\phi)}, \quad \varepsilon_6 = \frac{\Delta}{2} - \frac{\Delta}{2\cos(\phi)}, \quad \varepsilon_7 = \Delta, \end{aligned} \quad (33)$$

where $\phi = \tan^{-1}\left(\frac{4J}{\sqrt{2}\Delta}\right)$, with $-\frac{\pi}{2} \leq \phi \leq \frac{\pi}{2}$. While the corresponding eigenvector are given in the Appendix eq.(A.4).

After performing the partial trace over \mathbf{s} in eq.(4), we obtain the reduced operator \mathbf{W}_r , which has the same structure to the eq.(15), in terms of natural basis $\{|\sigma_1, \sigma_2\rangle\}$. Whereas, w_1 , w_2 and w_3 can be expressed by

$$\begin{aligned} w_1 &= \frac{1}{2}e^{-\frac{\beta\Delta}{2}} \cosh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) - \frac{1}{2}e^{-\frac{\beta\Delta}{2}} \sinh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) \cos(\phi) + \cosh(\beta J) + e^{\beta\Delta} + \frac{1}{2}e^{-\beta\Delta}, \\ w_2 &= e^{-\frac{\beta\Delta}{2}} \cosh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) + e^{-\frac{\beta\Delta}{2}} \sinh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) \cos(\phi) + 2\cosh(\beta J), \\ w_3 &= 3, \end{aligned} \quad (34)$$

where for the null magnetic field, we have the symmetry $w_4 = w_1$.

On the other hand, the operator $\tilde{\mathbf{W}}$ is given by eq.(28), and its elements can be written as a function of

$$\tilde{w}_1 = e^{-\beta(-\tilde{J}_0 - \frac{\tilde{\Delta}}{4})}, \quad \tilde{w}_2 = e^{-\beta(-\tilde{J}_0 + \frac{\tilde{\Delta}}{4} - \frac{\tilde{J}}{2})}, \quad \tilde{w}_3 = e^{-\beta(-\tilde{J}_0 + \frac{\tilde{\Delta}}{4} + \frac{\tilde{J}}{2})}, \quad (35)$$

for the limiting case of the null magnetic field, we have the following relation $\tilde{w}_4 = \tilde{w}_1$.

Hereafter, we can impose that the elements must be identical for both operators. Analogous to the previous case, we have three parameters \tilde{J}_0 , \tilde{J} , and $\tilde{\Delta}$ to be determined and three algebraic equations. Then, we can obtain all unknown parameters \tilde{J}_0 , \tilde{J} and $\tilde{\Delta}$ in a transformed system as a function of decorated Hamiltonian parameters J and Δ . Thus, solving the algebraic system we have

$$\tilde{J}_0 = \frac{1}{4\beta} \ln[w_1^2 w_2 w_3], \quad \tilde{\Delta} = \frac{1}{\beta} \ln\left(\frac{w_1^2}{w_2 w_3}\right), \quad \tilde{J} = \frac{1}{\beta} \ln\left(\frac{w_2}{w_3}\right). \quad (36)$$

Note that, this result can also be obtained directly from eqs. (31) assuming $w_1 = w_4$. For the case of $w_2 = w_3$, we have $\tilde{J} = 0$, which corresponds to the classical decoration transformation.

Therefore, to transform the isotropic Heisenberg model into another effective isotropic Heisenberg model, we need to impose the following relation

$$w_1 w_4 = w_2^2. \quad (37)$$

The Isotropic ($\Delta = J$) Heisenberg model under null magnetic field can be mapped into another effective isotropic ($\tilde{\Delta} = \tilde{J}$) Heisenberg model ($\text{XXX} \leftrightarrow \text{XXX}$), although this symmetry is breaking when the model is under magnetic field. Thus, the isotropic ($\Delta = J$) Heisenberg model will be mapped into another effective anisotropic ($\tilde{\Delta} \neq \tilde{J}$) Heisenberg model ($\text{XXX} \leftrightarrow \text{XXZ}$). Several variants of Heisenberg type models can be mapped into another effective Heisenberg type models.

Not all models can be mapped into another model with its original symmetry. Such as the XY model, this model cannot be mapped into another effective XY model, but into a more general XYZ model ($\text{XY} \leftrightarrow \text{XYZ}$), not discussed here[42].

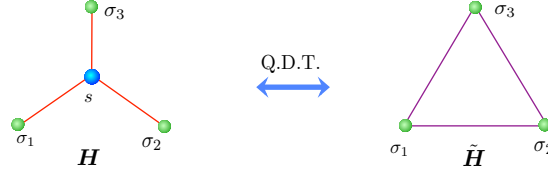


Figure 2: Schematic representation of star-triangle quantum decoration transformation. Where s corresponds to decorated spin, while σ_1 , σ_2 and σ_3 correspond to Heisenberg spins, H (\tilde{H}) corresponds to decorated (effective) Hamiltonian respectively.

3. Star-triangle quantum decoration transformation

Now let us consider another quite interesting quantum system with 3-leg star, a decorated operator is located in the center of the star denoted by s operator called "decorated operator", and in each leg is distributed the operators σ_1 , σ_2 and σ_3 .

Defining the operator $\mathbf{W} = e^{-\beta \mathbf{H}}$, where \mathbf{H} is the Hamiltonian of decorated system illustrated on left side of fig.2. Assuming the Hamiltonian \mathbf{H} 's eigenvalues as ε_n , and the corresponding orthonormal eigenvectors by $|\eta_n\rangle$, with $n = \{1, \dots, \dim(H)\}$.

Explicitly, the operator \mathbf{W} can be expressed by

$$\mathbf{W} = e^{-\beta \mathbf{H}} = \sum_{n=1}^{\dim(H)} e^{-\beta \varepsilon_n} |\eta_n\rangle \langle \eta_n|. \quad (38)$$

Multiplying both sides of operator \mathbf{W} by identity operator $\mathbf{1} = \sum_{s, \{\sigma_i\}} |s, \{\sigma_i\}\rangle \langle s, \{\sigma_i\}|$, and using for convenience the following notation $\{\sigma_i\} = \{\sigma_1, \sigma_2, \sigma_3\}$, the summation runs over s , σ_1 , σ_2 , and σ_3 . Thus, the operator \mathbf{W} becomes

$$\mathbf{W} = \sum_{n=1}^{\dim(H)} \sum_{s, \{\sigma_i\}} \sum_{s', \{\sigma'_i\}} e^{-\beta \varepsilon_n} c_{s, \{\sigma_i\}}^{n*} c_{s', \{\sigma'_i\}}^n |s, \{\sigma_i\}\rangle \langle s', \{\sigma'_i\}|, \quad (39)$$

where the scalar products are $c_{s, \{\sigma_i\}}^n = \langle \eta_n | s, \{\sigma_i\} \rangle$ and $c_{s, \{\sigma_i\}}^{n*} = \langle s, \{\sigma_i\} | \eta_n \rangle$.

Performing the partial trace over s , given by eq (4), we have the reduced operator

$$\mathbf{W}_r = \sum_{n=1}^{\dim(H)} \sum_{s, \{\sigma_i\}} \sum_{\{\sigma'_i\}} e^{-\beta \varepsilon_n} c_{s, \{\sigma_i\}}^{n*} c_{s', \{\sigma'_i\}}^n | \{\sigma_i\} \rangle \langle \{\sigma'_i\} |, \quad (40)$$

with the scalar products given by $| \{\sigma_i\} \rangle = \langle s | s, \{\sigma_i\} \rangle$ and $\langle \{\sigma_i\} | = \langle s, \{\sigma_i\} | s \rangle$. Using this representation, we can rewrite the elements of reduced operator \mathbf{W}_r conveniently as

$$r_{\{\sigma_i\}; \{\sigma'_i\}} = \sum_{n=1}^{\dim(H)} \sum_s e^{-\beta \varepsilon_n} c_{s, \{\sigma_i\}}^{n*} c_{s, \{\sigma'_i\}}^n. \quad (41)$$

On the other hand, the transformed system is represented schematically on the right side of fig.2. Analogously, we define another operator $\tilde{\mathbf{W}}$, as $\tilde{\mathbf{W}} = e^{-\beta \tilde{\mathbf{H}}}$, where $\tilde{\mathbf{H}}$ is the Hamiltonian of the transformed system called as effective Hamiltonian.

Multiplying the operator $\tilde{\mathbf{W}}$ by the identity operator $\mathbf{1} = \sum_{\{\sigma_i\}} e^{-\beta \tilde{\mathbf{H}}} | \{\sigma_i\} \rangle \langle \{\sigma_i\} |$, we have

$$\tilde{\mathbf{W}} = \sum_{n=1}^4 \sum_{\{\sigma_i\}} \sum_{\{\sigma'_i\}} e^{-\beta \tilde{\varepsilon}_n} \tilde{c}_{\{\sigma_i\}}^{n*} \tilde{c}_{\{\sigma'_i\}}^n | \{\sigma_i\} \rangle \langle \{\sigma'_i\} |, \quad (42)$$

with scalar products being $\tilde{c}_{\{\sigma_i\}}^n = \langle \zeta_n | \{\sigma_i\} \rangle$ and $\tilde{c}_{\{\sigma_i\}}^{n*} = \langle \{\sigma_i\} | \zeta_n \rangle$. Thus, the elements of $\tilde{\mathbf{W}}$ are given by

$$\tilde{r}_{\{\sigma_i\}; \{\sigma'_i\}} = \sum_{n=1}^4 e^{-\beta \tilde{\varepsilon}_n} \tilde{c}_{\{\sigma_i\}}^{n*} \tilde{c}_{\{\sigma'_i\}}^n. \quad (43)$$

After the partial trace is performed in \mathbf{s} , the elements of $\tilde{\mathbf{W}}$ must be identical to \mathbf{W}_r . Certainly, this is a natural generalization of a classical star-triangle decoration transformation[1]. This means that, all elements of \mathbf{W}_r and $\tilde{\mathbf{W}}$ composed only of σ_1 , σ_2 and σ_3 must satisfy the following relation

$$r_{\{\sigma_i\};\{\sigma'_i\}} = \tilde{r}_{\{\sigma_i\};\{\sigma'_i\}}. \quad (44)$$

Surely, this result can be straightforwardly generalized for a n -leg star-polygon transformation, we just need to extend our spin notation to $\{\sigma_i\} = \{\sigma_1, \sigma_2, \dots, \sigma_n\}$. Although, this transformation will involve next nearest and further nearest neighbor coupling terms, similar to that discussed in reference [11].

In the following subsections, we will give a couple of examples to show how this transformation works.

3.1. Quantum decoration transformation for spin- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ model

Let us transform a typical star shape system, composed of spin-1/2 Heisenberg model. Whose Hamiltonian of star model can be considered as decorated system with spin- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ model, the first spin corresponds to the central spin, thus we have

$$\mathbf{H} = -J[s^x(\sigma_1^x + \sigma_2^x + \sigma_3^x) + s^y(\sigma_1^y + \sigma_2^y + \sigma_3^y)] - \Delta s^z(\sigma_1^z + \sigma_2^z + \sigma_3^z), \quad (45)$$

where σ_i^α and s^α (with $\alpha = \{x, y, z\}$ and $i = \{1, 2, 3\}$) are spin-1/2 operators, as well as J and Δ are Heisenberg parameters as defined in eq.(10).

To diagonalize the Hamiltonian (45), we can express the Hamiltonian in natural basis $\{|s, \sigma_1, \sigma_2, \sigma_3\rangle\}$ as 16×16 matrix.

Therefore, the Hamiltonian (45) eigenvalues become

$$\begin{aligned} \varepsilon_1 = \varepsilon_2 = -\frac{3\Delta}{4}, \quad \varepsilon_3 = \varepsilon_4 = \varepsilon_5 = \varepsilon_6 = -\frac{\Delta}{4}, \quad \varepsilon_7 = \varepsilon_8 = \frac{\Delta}{4} \pm J, \\ \varepsilon_9 = \varepsilon_{10} = \varepsilon_{11} = \varepsilon_{12} = \frac{\Delta}{4} \pm \frac{J}{2}, \quad \varepsilon_{13} = \varepsilon_{14} = \varepsilon_{15} = \varepsilon_{16} = \frac{\Delta}{4} \pm \frac{\Delta}{2\cos(\phi)}, \end{aligned} \quad (46)$$

where $\phi = \tan^{-1}\left(\frac{\sqrt{3}J}{\Delta}\right)$ with $-\frac{\pi}{2} \leq \phi \leq \frac{\pi}{2}$.

The corresponding eigenvectors are expressed in Appendix eq.(A.5). Once we have calculated the partial trace using the eq.(40), we obtain the reduced operator \mathbf{W}_r as

$$\mathbf{W}_r = \begin{bmatrix} w_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{w_2+2w_3}{3} & \frac{w_2-w_3}{3} & \frac{w_2-w_3}{3} & 0 & 0 & 0 & 0 \\ 0 & \frac{w_2-w_3}{3} & \frac{w_2+2w_3}{3} & \frac{w_2-w_3}{3} & 0 & 0 & 0 & 0 \\ 0 & \frac{w_2-w_3}{3} & \frac{w_2-w_3}{3} & \frac{w_2+2w_3}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{w_2+2w_3}{3} & \frac{w_2-w_3}{3} & \frac{w_2-w_3}{3} & 0 \\ 0 & 0 & 0 & 0 & \frac{w_2-w_3}{3} & \frac{w_2+2w_3}{3} & \frac{w_2-w_3}{3} & 0 \\ 0 & 0 & 0 & 0 & \frac{w_2-w_3}{3} & \frac{w_2-w_3}{3} & \frac{w_2+2w_3}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_1 \end{bmatrix}, \quad (47)$$

where the elements can be written as a function of

$$w_1 = e^{-\frac{\beta\Delta}{4}} \cosh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) - e^{-\frac{\beta\Delta}{4}} \sinh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) \cos(\phi) + e^{\frac{3\beta\Delta}{4}}, \quad (48)$$

$$w_2 = e^{-\frac{\beta\Delta}{4}} \cosh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) + e^{-\frac{\beta\Delta}{4}} \sinh\left(\frac{\beta\Delta}{2\cos(\phi)}\right) \cos(\phi) + e^{-\frac{\beta\Delta}{4}} \cosh(\beta J), \quad (49)$$

$$w_3 = e^{-\frac{\beta\Delta}{4}} \cosh\left(\frac{\beta J}{2}\right) + e^{\frac{\beta\Delta}{4}}. \quad (50)$$

On the other hand, the effective spin-1/2 Heisenberg model in a triangle system can be expressed by

$$\tilde{\mathbf{H}} = -\tilde{J}_0 - \tilde{J}(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + \sigma_2^x\sigma_3^x + \sigma_2^y\sigma_3^y + \sigma_3^x\sigma_1^x + \sigma_3^y\sigma_1^y) - \tilde{\Delta}(\sigma_1^z\sigma_2^z + \sigma_2^z\sigma_3^z + \sigma_3^z\sigma_1^z), \quad (51)$$

where \tilde{J}_0 is a ‘‘constant’’ energy, \tilde{J} is the exchange parameter between σ_1 , σ_2 and σ_3 in xy axes, $\tilde{\Delta}$ represents the exchange parameter in z axis.

Thus, the elements of matrix $\tilde{\mathbf{W}}$ is given by (42), which can be written as a function of,

$$\tilde{w}_1 = e^{\beta(\tilde{J}_0 + \frac{3\tilde{\Delta}}{4})}, \quad \tilde{w}_2 = e^{\beta(\tilde{J}_0 + \tilde{J} - \frac{\tilde{\Delta}}{4})}, \quad \tilde{w}_3 = e^{\beta(\tilde{J}_0 - \frac{\tilde{J}}{2} - \frac{\tilde{\Delta}}{4})}. \quad (52)$$

Analogously to the previous case, imposing the condition $\tilde{w}_1 = w_1$, $\tilde{w}_2 = w_2$, $\tilde{w}_3 = w_3$, we find an algebraic systems equations. Solving the system equations, we have

$$\tilde{J}_0 = \frac{1}{4\beta} \ln [w_1 w_2 w_3^2], \quad \tilde{\Delta} = \frac{1}{3\beta} \ln \left(\frac{w_1^3}{w_2 w_3^2} \right), \quad \tilde{J} = \frac{2}{3\beta} \ln \left(\frac{w_2}{w_3} \right). \quad (53)$$

For the case of $w_2 = w_3$, the eq. (47) becomes a diagonal matrix, because $\tilde{J} = 0$ or $J = 0$ dropping to classical decoration transformation.

3.2. Quantum decoration transformation for spin- $(1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ model

Here, we study a typical star structure with central spin-1, and other spins are spin-1/2 particles. Thus, the system is described by the Hamiltonian of spin- $(1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ model, which is given by

$$\mathbf{H} = -[Js^x(\sigma_1^x + \sigma_2^x + \sigma_3^x) + Js^y(\sigma_1^y + \sigma_2^y + \sigma_3^y) + \Delta s^z(\sigma_1^z + \sigma_2^z + \sigma_3^z)], \quad (54)$$

writing the Hamiltonian (54) in standard basis $\{|s, \sigma_1, \sigma_2, \sigma_3\rangle\}$, we have a matrix with dimension 24×24 , this matrix becomes large enough to write explicitly with several zero elements.

For the anisotropic case ($\Delta \neq J$), the eigenvalues of the Hamiltonian (54) involve cubic algebraic equations, one can solve this one analytically. However, here we only focus on the isotropic case ($\Delta = J$), and its solution just involves quadratic algebraic equations.

Furthermore, using eq.(40), we can obtain the reduced operator \mathbf{W}_r , which has exactly the same structure to the eq.(47). Then, only w_1 , w_2 and w_3 are defined by the following expressions

$$w_1 = \frac{1}{2}e^{-\frac{\beta 5\Delta}{2}} + \frac{3}{2}e^{\frac{\beta 3\Delta}{2}} + e^{-\beta\Delta}, \quad w_2 = \frac{1}{6}e^{-\frac{\beta 5\Delta}{2}} + \frac{1}{2}e^{\frac{\beta 3\Delta}{2}} + \frac{1}{2}e^{-\beta\Delta} + \frac{1}{3}e^{\frac{\beta\Delta}{2}}, \quad w_3 = \frac{1}{2}e^{-\beta\Delta} + e^{\frac{\beta\Delta}{2}}. \quad (55)$$

On the other side, the Hamiltonian of effective spin-1/2 Heisenberg model in a triangle system is given by (51), because the effective model is exactly the same to the previous application.

Imposing the condition $\tilde{\mathbf{W}} = \mathbf{W}_r$, whose matrix structure is given by (47). Therefore, the effective parameters are given by (53), and the explicit expressions of w_1 , w_2 and w_3 are given by eq.(55).

It is quite remarkable the extension of decoration transformation for quantum spin models since most of the real materials could be well described by Heisenberg type models. Furthermore, the quantum decoration transformation could be exactly applied to small quantum systems, such as coupled spin systems[36, 37, 38, 39] among other models.

In addition, the decoration transformation can be applied, for several other models. However, we must be careful in applying this approach, because not all Hamiltonians satisfy its corresponding original Hamiltonian symmetry. It is worth to mention also, that this transformation cannot be applied naively for lattice models, due to non-commuting operators.

4. Decoration transformation for quantum lattice models

Obviously, the decoration transformation discussed previously cannot be applied naively for quantum spin lattice models. Contrary to the classical spin decoration transformation which can be applied exactly to lattice spin models.

4.1. Quantum decoration transformation correction using Zassenhaus formula

For quantum decoration transformation, the operators are no longer commutative operators, because immediately arises a second nearest neighbor and further nearest neighbors, leading to a very cumbersome Hamiltonian turning its solution in a tricky task, and the spirit of the decoration transformation is completely lost.

For instance, without lose its generality, let us consider a quantum chain model given by

$$\mathcal{H} = \sum_{i=1}^{2N} \mathbf{H}_{i,i+1} = \mathbf{H}_{1,2} + \mathbf{H}_{2,3} + \mathbf{H}_{3,4} \cdots, \quad (56)$$

with open boundary condition and $2N + 1$ sites, and assuming all even sites as decorated spins.

Therefore, grouping the Hamiltonian as follows

$$\mathcal{H} = (\mathbf{H}_{1,2} + \mathbf{H}_{2,3}) + (\mathbf{H}_{3,4} + \mathbf{H}_{4,5}) + (\mathbf{H}_{5,6} + \mathbf{H}_{6,7}) + \cdots, \quad (57)$$

$$= \mathbf{H}_{1,3} + \mathbf{H}_{3,5} + \mathbf{H}_{5,7} + \cdots, \quad (58)$$

denoting $\mathbf{H}_{2i-1,2i+1} = \mathbf{H}_{2i-1,2i} + \mathbf{H}_{2i,2i+1}$. In this notation all even sites are considered as decorated spins, then formally the system Hamiltonian becomes

$$\mathcal{H} = \sum_{i=1}^N \mathbf{H}_{2i-1,2i+1}. \quad (59)$$

Now we want to apply the decoration transformation for whole lattice system, then we can use the Zassenhaus formula[43] ($e^{\mathbf{X}+\mathbf{Y}} = e^{\mathbf{X}}e^{\mathbf{Y}} \prod_{n=2}^{\infty} e^{P_n(\mathbf{X},\mathbf{Y})}$ where $P_n(\mathbf{X},\mathbf{Y})$ is a Lie polynomial \mathbf{X} and \mathbf{Y} of degree n) which is a dual representation of the well known, Baker-Campbell-Hausdorff theorem[44] ($e^{\mathbf{X}}e^{\mathbf{Y}} = e^{\mathbf{Z}}$, with $\mathbf{Z} = \mathbf{X} + \mathbf{Y} + \sum_{m=2}^{\infty} Q_m(\mathbf{X},\mathbf{Y})$ where $Q_m(\mathbf{X},\mathbf{Y})$ is a Lie polynomial in \mathbf{X} and \mathbf{Y} of degree m).

Now let us define the following system operator $\mathbb{W} = e^{-\beta\mathcal{H}}$. Using the Zassenhaus formula[43] with N operators to obtain the correction of decoration transformation, as described in Appendix C, up to second order term. Thus, the equivalent reduced operator \mathbb{W}_r , after some algebraic manipulation can be expressed by the following relation,

$$\mathbb{W}_r = e^{-\beta(\sum_{i=1}^N \tilde{\mathbf{H}}_{2i-1,2i+1})} + \frac{\beta^2}{2} \sum_{j=1}^{N-1} \left([\tilde{\mathbf{H}}_{2j-1,2j+1}, \tilde{\mathbf{H}}_{2j+1,2j+3}] - [\mathbf{H}'_{2j-1,2j+1}, \mathbf{H}''_{2j+1,2j+3}] \right) + \mathcal{O}(\beta^3), \quad (60)$$

where the second term of eq. (60) corresponds to the correction in order β^2 .

For most of the Heisenberg model, the second order term is identically null, because it involves the only bilinear like power operators. However, for non-bilinear operators the second order coefficient of β^2 could be relevant.

At first glance, one could believe to include this term to correct our results of decoration transformation. But, we face a serious problem, because this term includes three nearest neighbor couplings. Consequently, the spirit of decoration transformation fails, and we cannot to map into another effective Heisenberg model with only nearest neighbor coupling term (a simple structure). However, one can use the correction term just to quantify the validity of our result.

Similarly, for standard Heisenberg model the third order correction (β^3) will be null because the Heisenberg spins are traceless. Then, this term also does not contribute, unless for non-bilinear like Hamiltonians, this term could be relevant. One can find an expression similar to eq. (60), but the result will be useless for decoration transformation, because it involves next nearest neighbor and further nearest neighbor couplings.

Another interesting way to prove this correction can be also find using the cumulant expansion [41], or even alternatively following the series expansion developed in reference [45], particularly the last one could be useful for higher order terms.

Note that, for higher dimension the spin models can be mapped in a similar way, although the coupling terms could be a bit more cumbersome task.

4.2. Heisenberg chain as a decorated Heisenberg chain

As a first application let us consider the spin-1/2 Heisenberg chain, to verify the quantum decoration transformation approach. Let us consider a spin- $\frac{1}{2}$ Heisenberg chain with $N' = 2N$ sites, and periodic boundary condition, given by the following Hamiltonian

$$\mathcal{H} = - \sum_{i=1}^N \left\{ J (\sigma_{2i-1}^x s_{2i}^x + \sigma_{2i-1}^y s_{2i}^y + s_{2i}^x \sigma_{2i+1}^x + s_{2i}^y \sigma_{2i+1}^y) + \Delta \sigma_{2i-1}^z s_{2i}^z + \Delta s_{2i}^z \sigma_{2i+1}^z \right\}, \quad (61)$$

where we label only for convenience the even site as $s_{2i} = \{s_{2i}^x, s_{2i}^y, s_{2i}^z\}$ and the odd site by $\sigma_{2i+1} = \{\sigma_{2i+1}^x, \sigma_{2i+1}^y, \sigma_{2i+1}^z\}$, but both of them are spin- $\frac{1}{2}$ particles. Thus, we will call the spin s_{2i} as "decorated" spin. Performing the decoration transformation presented in the previous section, the effective Hamiltonian becomes

$$\tilde{\mathcal{H}} = -N\tilde{J}_0 - \sum_{j=1}^N \left\{ \tilde{J} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \tilde{\Delta} \sigma_j^z \sigma_{j+1}^z \right\}, = -N\tilde{J}_0 + \tilde{\mathcal{H}}_{ex}. \quad (62)$$

where $\tilde{\mathcal{H}}_{ex}$ corresponds to standard Heisenberg model with effective parameters \tilde{J}_0 , \tilde{J} and $\tilde{\Delta}$ which are given by eq. (31).

This model can be solved numerically for finite size chain, through exact numerical diagonalization. We choose this approach in order to confront the exact numerical results and using the quantum decoration transformation approach.

J	T	$(N = 4) \tilde{f}^{(4)}$	$(N' = 8) f^{(8)}$	$f^{(8)} - \tilde{f}^{(4)}$	$(N = 8) \tilde{f}^{(8)}$	$(N' = 16) f^{(16)}$	$f^{(16)} - \tilde{f}^{(8)}$
0.1	0.1	-0.2586958	-0.2611776	2.4819×10^{-3}	-0.2543836	-0.2568705	2.4870×10^{-3}
	0.2	-0.2718840	-0.2742885	2.4045×10^{-3}	-0.2669289	-0.2693436	2.4147×10^{-3}
	0.3	-0.3040827	-0.3059479	1.8652×10^{-3}	-0.3024891	-0.3043023	1.8133×10^{-3}
	0.4	-0.3518063	-0.3531251	1.3189×10^{-3}	-0.3513949	-0.3526862	1.2913×10^{-3}
	0.5	-0.4073722	-0.4083200	0.9479×10^{-3}	-0.4072546	-0.4081909	0.9364×10^{-3}
0.5	0.1	-0.2651621	-0.3181141	5.2952×10^{-2}	-0.2604893	-0.3134708	5.29815×10^{-2}
	0.2	-0.2820743	-0.3304106	4.83363×10^{-2}	-0.2793074	-0.3272538	4.79464×10^{-2}
	0.3	-0.318616	-0.3565787	3.79625×10^{-2}	-0.3180631	-0.3554160	4.79464×10^{-2}
	0.4	-0.3674966	-0.3957681	2.82715×10^{-2}	-0.3673978	-0.3954009	2.80031×10^{-2}
	0.5	-0.4227335	-0.4439272	2.11937×10^{-2}	-0.4227128	-0.4438067	2.10939×10^{-2}
1.0	0.1	-0.3200886	-0.4565879	1.36499×10^{-1}	-0.311581	-0.4476710	1.3609×10^{-1}
	0.2	-0.3381643	-0.4619391	1.23775×10^{-1}	-0.334471	-0.4571226	1.2265×10^{-1}
	0.3	-0.3727897	-0.4775811	1.04791×10^{-1}	-0.371347	-0.4755115	1.0416×10^{-1}
	0.4	-0.4182362	-0.5036855	8.54493×10^{-2}	-0.4175997	-0.5028689	8.5269×10^{-2}
	0.5	-0.4707678	-0.5388776	6.81098×10^{-2}	-0.4704224	-0.5385579	6.8136×10^{-2}

Table 1: Free energy as a function of temperature for fixed parameter $\Delta = 1.0$.

Therefore, we can find the free energy per site ($N' = 2N$) as

$$f^{(2N)} = -\frac{1}{2N\beta} \ln(Z_{2N}), \quad \text{and} \quad \tilde{f}^{(N)} = -\frac{\tilde{J}_0}{2} - \frac{1}{2N\beta} \ln(\tilde{Z}_{ex,N}), \quad (63)$$

where $Z_{2N} = \text{tr}(e^{-\beta\mathcal{H}})$ and $\tilde{Z}_{ex,N} = \text{tr}(e^{-\beta\tilde{\mathcal{H}}_{ex}})$, are the partition functions of Hamiltonian (61) and (62) respectively.

In table 1, we show the numerical results for fixed parameters $J = 0.1$ and $\Delta = 1.0$ (a quasi-Ising model), comparing for a range of temperatures given in the first column, the second column presents the free energy per site $\tilde{f}^{(4)}$ for effective Heisenberg model with $N = 4$, the third column shows the free energy $f^{(8)}$ numerical result for ($N' = 2N = 8$), and in the fourth column is shown the difference between both free energies. Whereas the fifth column displays the free energy per site $\tilde{f}^{(8)}$ of effective lattice ($N = 8$), and in the sixth column, we show the original lattice free energy $f^{(16)}$ numerical result ($N' = 2N = 16$). In table 1, we observe the results are in agreement, and the effective free energy is slightly higher than original Heisenberg chain, this discrepancy was to be expected, because the method is only approximate. Notice that, the effective Heisenberg model only needs half sites compared to the original Hamiltonian. We have compared only in relatively low temperature region, this difference is more significant when the temperature decreases, whereas in the high temperature region both results are obviously accurate. Surely, this result could be valuable combining with numerical approaches. In table 1, we observe the numerical results for $J = 0.5$ is poorly accurate, as well as for $J = 1.0$ our results are even worse, because the quantum coupling is rather relevant.

The above process resembles a real-space renormalization-group transformation[46], because we are considering uniform spin-1/2 Heisenberg model. However, for mixed or real decorated Heisenberg model, the decorated transformation goes beyond the renormalization transformation.

More detailed analyses using this method would be interesting, but these analyses are out of the scope of this work.

4.3. Bond alternating Ising-Heisenberg chain

As a second application, let us consider the bond alternating Ising-Heisenberg chain early proposed by Lieb-Schultz-Mattis[47]. Certainly, this model cannot be mapped exactly into another effective model through classical decoration transformation. Although the quantum decoration transformation cannot be applied exactly, here we present an approximate solution for this model, in the limit of quasi Ising model.

The corresponding Hamiltonian that describes the Ising-Heisenberg model could be written in a similar way to eq.(59). Thus, the Hamiltonian is given by

$$\mathcal{H} = \sum_{i=1}^N \mathbf{H}_{2i-1,2i+1}, \quad \text{where} \quad \mathbf{H}_{2i-1,2i+1} = -\Delta \sigma_{2i-1}^z \sigma_{2i}^z - J (s_{2i}^x \sigma_{2i+1}^x + s_{2i}^y \sigma_{2i+1}^y) - J_z s_{2i}^z \sigma_{2i+1}^z, \quad (64)$$

with periodic boundary condition. The eigenvalues of the Hamiltonian $\mathbf{H}_{2i-1,2i+1}$ in (64) are given by

$$\varepsilon_{1(2)} = \frac{-\Delta}{4} - \frac{J_z}{4}, \quad \varepsilon_{3(4)} = \frac{\Delta}{4} - \frac{J_z}{4}, \quad \varepsilon_{5(6)} = \frac{J_z}{4} - \frac{\Delta}{4 \cos \phi}, \quad \varepsilon_{7(8)} = \frac{J_z}{4} + \frac{\Delta}{4 \cos \phi}, \quad (65)$$

where $\phi = \arctan\left(\frac{2J}{\Delta}\right)$. Whereas the corresponding eigenvectors are

$$\begin{aligned} |u_{1(2)}\rangle &= |\pm, \pm, \pm\rangle, & |u_{3(4)}\rangle &= |\mp, \pm, \mp\rangle, \\ |u_{5(6)}\rangle &= \frac{\mp 1}{\sqrt{2}} \left(\sqrt{1 \pm \cos \phi} |+, -, -\rangle + |-, -, +\rangle \right), & |u_{7(8)}\rangle &= \frac{\mp 1}{\sqrt{2}} \left(\sqrt{1 \mp \cos \phi} |+, -, -\rangle + |-, -, +\rangle \right). \end{aligned} \quad (66)$$

Following the recipes in the previous section, we can obtain the reduced operator \mathbf{W}_r given by eq.(15), this reduced operator becomes just a diagonal matrix in a natural basis, because $w_3 = w_2$, as well as for null magnetic field we have $w_4 = w_1$. Thus, w_1 and w_2 are obtained using the eq.(65), as follows

$$\begin{aligned} w_1 &= e^{\beta(\frac{J_z+\Delta}{4})} + e^{-\beta\frac{J_z}{4}} \left[\cosh\left(\frac{\beta\Delta}{4\cos(\phi)}\right) + \cosh\left(\frac{\beta\Delta}{4\cos(\phi)}\right) \cos(\phi) \right], \\ w_2 &= e^{\beta(\frac{J_z-\Delta}{4})} + e^{-\beta\frac{J_z}{4}} \left[\cosh\left(\frac{\beta\Delta}{4\cos(\phi)}\right) - \cosh\left(\frac{\beta\Delta}{4\cos(\phi)}\right) \cos(\phi) \right]. \end{aligned} \quad (67)$$

The decorated model can be mapped into an effective spin-1/2 Ising model, given by

$$\tilde{\mathcal{H}} = -N\tilde{J}_0 - \tilde{\Delta} \sum_{i=1}^N \sigma_i \sigma_{i+1}. \quad (68)$$

Where the eigenvalues and eigenvectors of $H_{i,i+1} = -\tilde{J}_0 - \tilde{\Delta} \sigma_i \sigma_{i+1}$, read as

$$\tilde{\varepsilon}_{1(2)} = -\tilde{J}_0 - \frac{\tilde{\Delta}}{4} \longrightarrow |v_{1(2)}\rangle = |\pm\pm\rangle, \quad \tilde{\varepsilon}_{3(4)} = -\tilde{J}_0 + \frac{\tilde{\Delta}}{4} \longrightarrow |v_{3(4)}\rangle = |\pm\mp\rangle. \quad (69)$$

Obviously, the corresponding $\tilde{\mathbf{W}}$ operator is also a diagonal matrix, and each element is compared $w_i = \tilde{w}_i$. Thus, the effective parameters are related by

$$\tilde{J}_0 = \frac{1}{2\beta} \ln(w_1 w_2), \quad \tilde{\Delta} = \frac{2}{\beta} \ln\left(\frac{w_1}{w_2}\right). \quad (70)$$

The spin-1/2 Ising model is a well known model, which can be solved exactly through the transfer matrix approach. Here we skip the detailed solution of this model, and only we present the result of the model. The 2×2 transfer matrix can be constructed $\mathbf{V} = \begin{bmatrix} w_1 & w_2 \\ w_2 & w_1 \end{bmatrix}$, whose eigenvalue are given by $\Lambda_{\pm} = e^{\beta\tilde{J}_0} \left(e^{\beta\tilde{\Delta}/4} \pm e^{-\beta\tilde{\Delta}/4} \right)$. The partition function of effective Ising chain with spin-1/2, becomes

$$Z_N = \Lambda_+^N + \Lambda_-^N. \quad (71)$$

In the thermodynamic limit $N \rightarrow \infty$, the free energy is expressed by

$$f = -\frac{\tilde{J}_0}{2} - \frac{1}{2\beta} \ln \left(e^{\beta\tilde{\Delta}/4} + e^{-\beta\tilde{\Delta}/4} \right) = -\frac{1}{2\beta} \ln(w_1 + w_2). \quad (72)$$

The free energy given by (72) is an approximate result for Hamiltonian (64), which is more consistent only for small J . Thus, this result in the limit of $J \rightarrow 0$ must be well described by

$$f = -\frac{1}{2\beta} \ln \left(2e^{\frac{\beta J_z}{4}} \cosh\left(\frac{\beta\Delta}{4}\right) + 2e^{-\frac{\beta J_z}{4}} \cosh\left(\frac{\beta\Delta}{4} + \frac{\beta J^2}{2\Delta}\right) \right). \quad (73)$$

The thermodynamics solution of bond alternating Ising-Heisenberg chain is less studied, and this analysis will be discussed elsewhere.

The ground state energy and spectral analysis of the Hamiltonian given by (64) has been discussed in reference [48, 49]. This model exhibits a phase transition at zero temperature when $J_z = 2J$. Our approach is unable to detect this phase transition at zero temperature, because our result is accurate in the limit of $J \rightarrow 0$, and in this limit our result exhibits a trivial phase transition at $J_z \rightarrow 0$.

5. Conclusion

Here we present a quantum version of decoration transformation and show how this transformation could be applied to Heisenberg type models. The present transformation is an exact mapping when only one decorated system composes the system. Here we propose an exact quantum decoration transformation and showing also interesting properties such as the persistence of symmetry such as (e.g. XXX decorated model \leftrightarrow XXX effective model), and the symmetry breaking during this transformation (e.g. XXX decorated model \leftrightarrow XXZ effective model).

This transformation could be useful to demonstrate the equivalence between two quantum spin models. In this work, we present some examples, such spin-1/2 Heisenberg model, and mixed spin-(1,1/2) Heisenberg model. Unfortunately, the quantum spin decoration transformation cannot be used to map exactly into another quantum spin lattice model, because the operators are non-commutative. However, in the "classical" limit it could be possible to perform a mapping to establish the equivalence between two quantum lattice spin models. To study the validity of this approach for quantum spin lattice model, we use the Zassenhaus formula and show the correction of quantum decoration transformation, when it is applied to the lattice spin models. The correction involves second nearest neighbor, and further nearest neighbor coupling into a cumbersome task to establish the equivalence between both lattices. This correction gives us a valuable information about its contribution, for most of the Heisenberg type models, this one could be irrelevant at least up to the third order of correction.

We applied to finite size Heisenberg chain and compared numerically our result with its exact numerical result, and our result is consistent. It is worth to mention that the difference of numerical result is almost independent of the number of sites. Similarly, we also applied to bond alternating Ising-Heisenberg chain, obtaining an approximate result. This result is accurate in the limit of weak xy anisotropy coupling ($J \rightarrow 0$) of bond alternating Ising-Heisenberg model.

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Appendix A. Explicit representation of the Hamiltonians

In this Appendix we present some Hamiltonians explicitly in its natural basis:

1. Spin- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ XXZ Hamiltonian \mathbf{H} in natural basis $\{|s, \sigma_1, \sigma_2\rangle\}$ becomes,

$$\mathbf{H} = \begin{bmatrix} -\frac{\Delta}{2} - \frac{h_1}{2} - h & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{h_1}{2} & 0 & -\frac{J}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{h_1}{2} & -\frac{J}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & \frac{\Delta}{2} - \frac{h_1}{2} + h & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\Delta}{2} + \frac{h_1}{2} - h & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & -\frac{J}{\sqrt{2}} & \frac{h_1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{J}{\sqrt{2}} & 0 & \frac{h_1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\Delta}{2} + \frac{h_1}{2} + h \end{bmatrix}. \quad (\text{A.1})$$

2. Spin- $(1, \frac{1}{2}, \frac{1}{2})$ XXZ Hamiltonian in natural basis $\{|s, \sigma_1, \sigma_2\rangle\}$, becomes a 12×12 matrix. The matrix \mathbf{H} can be obtained straightforwardly, as a composition of block matrices

$$\mathcal{H}_2 = \mathcal{H}_{-2} = [-\Delta],$$

$$\mathcal{H}_1 = \begin{bmatrix} 0 & 0 & \frac{-J}{\sqrt{2}} \\ 0 & 0 & \frac{-J}{\sqrt{2}} \\ \frac{-J}{\sqrt{2}} & \frac{-J}{\sqrt{2}} & \Delta \end{bmatrix}, \quad \mathcal{H}_{-1} = \begin{bmatrix} \Delta & \frac{-J}{\sqrt{2}} & \frac{-J}{\sqrt{2}} \\ \frac{-J}{\sqrt{2}} & 0 & 0 \\ \frac{-J}{\sqrt{2}} & 0 & 0 \end{bmatrix}, \quad \mathcal{H}_0 = \begin{bmatrix} 0 & \frac{-J}{\sqrt{2}} & \frac{-J}{\sqrt{2}} & 0 \\ \frac{-J}{\sqrt{2}} & 0 & 0 & \frac{-J}{\sqrt{2}} \\ \frac{-J}{\sqrt{2}} & 0 & 0 & \frac{-J}{\sqrt{2}} \\ 0 & \frac{-J}{\sqrt{2}} & \frac{-J}{\sqrt{2}} & 0 \end{bmatrix}. \quad (\text{A.2})$$

Therefore, the Hamiltonian (32) can be expressed as follows

$$\mathbf{H} = \mathcal{H}_2 \oplus \mathcal{H}_1 \oplus \mathcal{H}_0 \oplus \mathcal{H}_{-1} \oplus \mathcal{H}_{-2}. \quad (\text{A.3})$$

The eigenvalues is given in (33), and the eigenvectors of the Hamiltonian (32) are given by

$$\begin{aligned}
|\eta_1\rangle &= |1,+,+\rangle, & |\eta_{12}\rangle &= |-1,-,-\rangle. \\
|\eta_2\rangle &= \frac{1}{2} \left(|1,+, -\rangle + |1,-, +\rangle - \sqrt{2}|0,+, +\rangle \right), & |\eta_9\rangle &= \frac{1}{2} \left(|-1,+, -\rangle + |-1,-, +\rangle - \sqrt{2}|0,-, -\rangle \right), \\
|\eta_3\rangle &= \frac{1}{2} \left(|1,+, -\rangle + |1,-, +\rangle + \sqrt{2}|0,+, +\rangle \right), & |\eta_{10}\rangle &= \frac{1}{2} \left(|-1,+, -\rangle + |-1,-, +\rangle + \sqrt{2}|0,-, -\rangle \right), \\
|\eta_4\rangle &= \frac{1}{\sqrt{2}} (|1,-, +\rangle - |1,+, -\rangle), & |\eta_{11}\rangle &= \frac{1}{\sqrt{2}} (|-1,-, +\rangle - |-1,+, -\rangle), \\
|\eta_5\rangle &= \frac{1}{2} \left[\sqrt{1 - \cos(\phi)} (|0,+, -\rangle + |0,-, +\rangle) - \sqrt{1 + \cos(\phi)} (|1,-, -\rangle + |-1,+, +\rangle) \right], \\
|\eta_6\rangle &= \frac{1}{2} \left[\sqrt{1 + \cos(\phi)} (|0,+, -\rangle + |0,-, +\rangle) + \sqrt{1 - \cos(\phi)} (|1,-, -\rangle + |-1,+, +\rangle) \right], \\
|\eta_7\rangle &= \frac{1}{\sqrt{2}} (|1,-, -\rangle - |-1,+, +\rangle), & |\eta_8\rangle &= \frac{1}{\sqrt{2}} (|0,-, +\rangle - |0,+, -\rangle),
\end{aligned} \tag{A.4}$$

3. Spin- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ Hamiltonian(45) in natural $\{|s, \sigma_1, \sigma_2, \sigma_3\rangle\}$, can be expressed as 16×16 matrix, The eigenvalues of the Hamiltonian are expressed in (46), and the corresponding eigenvectors are given by

$$\begin{aligned}
|\eta_1\rangle &= |\downarrow, -, -, -\rangle, & |\eta_2\rangle &= |\uparrow, +, +, +\rangle, \\
|\eta_3\rangle &= \frac{1}{\sqrt{2}} (|\uparrow, +, -, +\rangle - |\uparrow, +, +, -\rangle), & |\eta_4\rangle &= \frac{1}{\sqrt{2}} (|\downarrow, -, -, +\rangle - |\downarrow, +, -, -\rangle), \\
|\eta_5\rangle &= \frac{1}{\sqrt{6}} (|\uparrow, +, +, -\rangle + |\uparrow, +, -, +\rangle - 2|\uparrow, -, +, +\rangle), & |\eta_6\rangle &= \frac{1}{\sqrt{6}} (|\downarrow, +, -, -\rangle + |\downarrow, -, +, -\rangle - 2|\downarrow, -, -, +\rangle), \\
|\eta_7\rangle &= \frac{1}{\sqrt{6}} (-|\uparrow, +, -, -\rangle - |\uparrow, -, +, -\rangle - |\uparrow, -, -, +\rangle + |\downarrow, +, +, -\rangle + |\downarrow, +, -, +\rangle + |\downarrow, -, +, +\rangle), \\
|\eta_8\rangle &= \frac{1}{\sqrt{6}} (|\uparrow, +, -, -\rangle + |\uparrow, -, +, -\rangle + |\uparrow, -, -, +\rangle + |\downarrow, +, +, -\rangle + |\downarrow, +, -, +\rangle + |\downarrow, -, +, +\rangle), \\
|\eta_9\rangle &= \frac{1}{2} (|\uparrow, +, -, -\rangle - |\uparrow, -, -, +\rangle - |\downarrow, +, +, -\rangle + |\downarrow, -, +, +\rangle), & |\eta_{11}\rangle &= \frac{1}{2} (|\uparrow, +, -, -\rangle - |\uparrow, -, -, +\rangle + |\downarrow, +, +, -\rangle - |\downarrow, -, +, +\rangle), \\
|\eta_{10}\rangle &= \frac{1}{2\sqrt{3}} (|\uparrow, +, -, -\rangle - 2|\uparrow, -, +, -\rangle + |\uparrow, -, -, +\rangle + |\downarrow, +, +, -\rangle - 2|\downarrow, +, -, +\rangle + |\downarrow, -, +, +\rangle), \\
|\eta_{12}\rangle &= \frac{1}{2\sqrt{3}} (|\uparrow, +, -, -\rangle - 2|\uparrow, -, +, -\rangle + |\uparrow, -, -, +\rangle - |\downarrow, +, +, -\rangle + 2|\downarrow, +, -, +\rangle - |\downarrow, -, +, +\rangle), \\
|\eta_{13}\rangle &= \frac{1}{\sqrt{6}} \left[\sqrt{3(1 + \cos(\phi))} |\uparrow, -, -, -\rangle - \sqrt{1 - \cos(\phi)} (|\downarrow, -, +, -\rangle + |\downarrow, +, -, -\rangle + |\downarrow, -, -, +\rangle) \right], \\
|\eta_{14}\rangle &= \frac{1}{\sqrt{6}} \left[\sqrt{3(1 + \cos(\phi))} |\downarrow, +, +, +\rangle - \sqrt{1 - \cos(\phi)} (|\uparrow, +, -, +\rangle + |\uparrow, +, +, -\rangle + |\uparrow, -, +, +\rangle) \right], \\
|\eta_{15}\rangle &= \frac{1}{\sqrt{6}} \left[\sqrt{3(1 - \cos(\phi))} |\uparrow, -, -, -\rangle + \sqrt{1 + \cos(\phi)} (|\downarrow, -, +, -\rangle + |\downarrow, +, -, -\rangle + |\downarrow, -, -, +\rangle) \right], \\
|\eta_{16}\rangle &= \frac{1}{\sqrt{6}} \left[\sqrt{3(1 - \cos(\phi))} |\downarrow, +, +, +\rangle + \sqrt{1 + \cos(\phi)} (|\uparrow, +, -, +\rangle + |\uparrow, +, +, -\rangle + |\uparrow, -, +, +\rangle) \right].
\end{aligned} \tag{A.5}$$

Appendix B. Diagonalization of the Hamiltonian XXZ with spin- $(1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Conveniently, the Hamiltonian (54) can be expressed using the conservation magnet momenta, resulting in block matrices as follows

$$\mathbf{H} = H_{\frac{5}{2}} \oplus H_{\frac{3}{2}} \oplus H_{\frac{1}{2}} \oplus H_{-\frac{1}{2}} \oplus H_{-\frac{3}{2}} \oplus H_{-\frac{5}{2}}. \tag{B.1}$$

Where, each block matrices can be described as follows:

1. For magnetic moment $m = \frac{5}{2}$, there is only one configuration $|+1, +, +, +\rangle$ for this magnetic moment, $H_{\frac{5}{2}} = [-\frac{3\Delta}{2}]$. Obviously, the corresponding eigenvalues and eigenvectors,

$$\varepsilon_1 = -\frac{3\Delta}{2}, \quad \rightarrow \quad |v_1\rangle = |+1, +, +, +\rangle. \tag{B.2}$$

2. For magnetic moment $m = \frac{3}{2}$, we have four states given by $\{|_{+1,+,+,-}\rangle, |_{+1,+,-,+}\rangle, |_{+1,-,+,+}\rangle, |_{0,+,+,+}\rangle\}$, and in this basis the block Hamiltonian can be expressed as

$$H_{\frac{3}{2}} = \begin{bmatrix} -\frac{\Delta}{2} & 0 & 0 & -\frac{J}{\sqrt{2}} \\ 0 & -\frac{\Delta}{2} & 0 & -\frac{J}{\sqrt{2}} \\ 0 & 0 & -\frac{\Delta}{2} & -\frac{J}{\sqrt{2}} \\ -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & 0 \end{bmatrix}. \quad (\text{B.3})$$

For the isotropic case $J = \Delta$, the eigenvalues and eigenvectors are given by

$$\begin{aligned} \varepsilon_2 &= -\frac{3\Delta}{2}, \rightarrow |v_2\rangle = \frac{1}{\sqrt{5}} \left(|_{+1,+,+,-}\rangle + |_{+1,+,-,+}\rangle + |_{+1,-,+,+}\rangle + \sqrt{2}|_{0,+,+,+}\rangle \right), \\ \varepsilon_3 &= \Delta, \rightarrow |v_3\rangle = \frac{1}{\sqrt{15}} \left(\sqrt{2}|_{+1,+,+,-}\rangle + \sqrt{2}|_{+1,+,-,+}\rangle + \sqrt{2}|_{+1,-,+,+}\rangle - 3|_{0,+,+,+}\rangle \right), \\ \varepsilon_4 &= -\frac{\Delta}{2} \rightarrow |v_4\rangle = \frac{1}{\sqrt{2}} (|_{+1,+,+,-}\rangle - |_{+1,+,-,+}\rangle), \\ \varepsilon_5 &= -\frac{\Delta}{2} \rightarrow |v_5\rangle = \frac{1}{\sqrt{2}} (|_{+1,+,+,-}\rangle - |_{+1,-,+,+}\rangle). \end{aligned}$$

3. For magnetic moment $m = \frac{1}{2}$, we have 7 states given by $\{|_{+1,+,+,-}\rangle, |_{+1,-,+,+}\rangle, |_{+1,-,+,+}\rangle, |_{0,+,+,-}\rangle, |_{0,+,+,-}\rangle, |_{0,-,+,+}\rangle, |_{-1,+,+,+}\rangle\}$, then the block Hamiltonian becomes

$$H_{\frac{1}{2}} = \begin{bmatrix} \frac{\Delta}{2} & 0 & 0 & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{\Delta}{2} & 0 & \frac{J}{\sqrt{2}} & 0 & -\frac{J}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{\Delta}{2} & 0 & \frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & 0 \\ -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & 0 & 0 & 0 & 0 & -\frac{J}{\sqrt{2}} \\ -\frac{J}{\sqrt{2}} & 0 & -\frac{J}{\sqrt{2}} & 0 & 0 & 0 & -\frac{J}{\sqrt{2}} \\ 0 & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & 0 & 0 & 0 & -\frac{J}{\sqrt{2}} \\ 0 & 0 & 0 & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & -\frac{J}{\sqrt{2}} & \frac{3\Delta}{2} \end{bmatrix}. \quad (\text{B.4})$$

Assuming $J = \Delta$, the corresponding eigenvalues and eigenvectors read as

$$\begin{aligned} \varepsilon_6 &= -\frac{3\Delta}{2}, \rightarrow |v_6\rangle = \frac{1}{\sqrt{10}} \{ |_{+1,+,+,-}\rangle + |_{+1,-,+,+}\rangle + |_{+1,-,+,+}\rangle + \\ &\quad + \sqrt{2}(|_{0,+,+,-}\rangle + |_{0,+,+,-}\rangle + |_{0,-,+,+}\rangle) + |_{-1,+,+,+}\rangle \}, \\ \varepsilon_7 &= -\frac{\Delta}{2}, \rightarrow |v_7\rangle = \frac{1}{\sqrt{6}} \left(|_{+1,+,+,-}\rangle - |_{+1,-,+,+}\rangle + \sqrt{2}(|_{0,+,+,-}\rangle - |_{0,-,+,+}\rangle) \right), \\ \varepsilon_8 &= -\frac{\Delta}{2}, \rightarrow |v_8\rangle = \frac{1}{3\sqrt{2}} \{ |_{+1,+,+,-}\rangle - 2|_{+1,-,+,+}\rangle + |_{+1,-,+,+}\rangle + \\ &\quad + \sqrt{2}(-|_{0,+,+,-}\rangle + 2|_{0,+,+,-}\rangle - |_{0,-,+,+}\rangle) \}, \\ \varepsilon_9 &= \Delta, \rightarrow |v_9\rangle = \frac{1}{\sqrt{6}} \left(\sqrt{2}(|_{+1,+,+,-}\rangle - |_{+1,-,+,+}\rangle) - (|_{0,+,+,-}\rangle - |_{0,-,+,+}\rangle) \right), \\ \varepsilon_{10} &= \Delta, \rightarrow |v_{10}\rangle = \frac{1}{3\sqrt{2}} \{ \sqrt{2}(|_{+1,+,+,-}\rangle - 2|_{+1,-,+,+}\rangle + |_{+1,-,+,+}\rangle) + |_{0,+,+,-}\rangle - 2|_{0,+,+,-}\rangle + |_{0,-,+,+}\rangle \}, \\ \varepsilon_{11} &= \Delta, \rightarrow |v_{11}\rangle = \frac{1}{3\sqrt{10}} \{ -4(|_{+1,+,+,-}\rangle + |_{+1,-,+,+}\rangle + |_{+1,-,+,+}\rangle) + \\ &\quad + \sqrt{2}(|_{0,+,+,-}\rangle + |_{0,+,+,-}\rangle + |_{0,-,+,+}\rangle) + 6|_{-1,+,+,+}\rangle \}, \\ \varepsilon_{12} &= \frac{5\Delta}{2}, \rightarrow |v_{12}\rangle = \frac{1}{3\sqrt{2}} \{ |_{+1,+,+,-}\rangle + |_{+1,-,+,+}\rangle + |_{+1,-,+,+}\rangle + \\ &\quad - \sqrt{2}(|_{0,+,+,-}\rangle + |_{0,+,+,-}\rangle + |_{0,-,+,+}\rangle) + 3|_{-1,+,+,+}\rangle \}. \end{aligned} \quad (\text{B.5})$$

4. For $m = -\frac{1}{2}$, we also have 7 states, and the Hamiltonian $H_{-\frac{1}{2}}$ is identical to $H_{\frac{1}{2}}$, but in different space spanned by $\{|-1,+,+,-\rangle, |-1,+,-,+\rangle, |-1,-,+,+\rangle, |0,-,-,+\rangle, |0,-,+,-\rangle, |0,+,+,-\rangle, |+1,-,-,-\rangle\}$. Therefore, the eigenvalues are identical to that given by $\varepsilon_6 \cdots \varepsilon_{12}$, and the corresponding eigenvectors also have same structure, using the symmetry $+\rightarrow -$ and $-\rightarrow +$, we can generate the corresponding eigenvectors.
5. For $m = -\frac{3}{2}$, we have an equivalent matrix structure to that $m = \frac{3}{2}$. Thus, the eigenvalues are identical to the case 2. Using the symmetry $+\rightarrow -$ and $-\rightarrow +$, we can construct the corresponding eigenvectors.
6. Whereas, for $m = -\frac{5}{2}$, we have an equivalent matrix structure to $m = \frac{5}{2}$, $H_{-\frac{5}{2}} = [-\frac{3\Delta}{2}]$, so the corresponding eigenvalues and eigenvectors are

$$\varepsilon_1 = -\frac{3\Delta}{2}, \quad \rightarrow \quad |v_{24}\rangle = |-1,-,-,-\rangle. \quad (\text{B.6})$$

Appendix C. Quantum decoration transformation correction

Using the Zassenhaus formula[43] with N operators, we can apply up to second order term, which reads as follows

$$\begin{aligned} \mathbb{W} &= e^{-\beta(\sum_{i=1}^N \mathbf{H}_{2i-1,2i+1})} = e^{-\beta \mathbf{H}_{1,3}} e^{-\beta(\mathbf{H}_{3,5} + \mathbf{H}_{5,7} + \cdots)} e^{-\beta^2[\mathbf{H}_{1,3}, \mathbf{H}_{3,5}]} \dots, \\ &= e^{-\beta \mathbf{H}_{1,3}} e^{-\beta \mathbf{H}_{3,5}} e^{-\beta(\mathbf{H}_{5,7} + \mathbf{H}_{7,9} + \cdots)} e^{-\beta^2[\mathbf{H}_{3,5}, \mathbf{H}_{5,7}]} e^{-\beta^2[\mathbf{H}_{1,3}, \mathbf{H}_{3,5}]} \dots, \\ &\vdots \end{aligned} \quad (\text{C.1})$$

After applying N times, we have the following expression

$$\mathbb{W} = \prod_{i=1}^N e^{-\beta \mathbf{H}_{2i-1,2i+1}} \prod_{j=N-1}^1 e^{-\beta^2[\mathbf{H}_{2j-1,2j+1}, \mathbf{H}_{2j+1,2j+3}]} \dots \quad (\text{C.2})$$

Therefore, the operator \mathbb{W} is valid at least up to $\mathcal{O}(\beta^2)$, then, simplifying eq.(C.2) we have

$$\mathbb{W} = \left(\prod_{i=1}^N e^{-\beta \mathbf{H}_{2i-1,2i+1}} \right) \left(1 - \frac{\beta^2}{2} \sum_{j=1}^{N-1} [\mathbf{H}_{2j-1,2j+1}, \mathbf{H}_{2j+1,2j+3}] \right) + \mathcal{O}(\beta^3), \quad (\text{C.3})$$

alternatively, even one can write as

$$\mathbb{W} = \prod_{i=1}^N e^{-\beta \mathbf{H}_{2i-1,2i+1}} - \frac{\beta^2}{2} \sum_{j=1}^{N-1} [\mathbf{H}_{2j-1,2j+1}, \mathbf{H}_{2j+1,2j+3}] + \mathcal{O}(\beta^3). \quad (\text{C.4})$$

Performing the partial trace over decorated spins (even sites), we have

$$\begin{aligned} \mathbb{W}_r &= \text{tr}_e \left(e^{-\beta(\sum_{i=1}^N \mathbf{H}_{2i-1,2i+1})} \right) \\ &= \text{tr}_e \left(\prod_{i=1}^N e^{-\beta \mathbf{H}_{2i-1,2i+1}} \right) - \frac{\beta^2}{2} \text{tr}_e \left(\sum_{j=1}^{N-1} [\mathbf{H}_{2j-1,2j+1}, \mathbf{H}_{2j+1,2j+3}] \right) + \mathcal{O}(\beta^3), \end{aligned} \quad (\text{C.5})$$

with tr_e we denote the partial trace over all even sites. After performing the partial trace over decorated spins, each element of the product contains just one even site. Thus, the partial trace over the even site can be distributed through the product,

$$\mathbb{W}_r = \prod_{i=1}^N \text{tr}_{2i} \left(e^{-\beta \mathbf{H}_{2i-1,2i+1}} \right) - \frac{\beta^2}{2} \sum_{j=1}^{N-1} \text{tr}_e ([\mathbf{H}_{2j-1,2j+1}, \mathbf{H}_{2j+1,2j+3}]) + \mathcal{O}(\beta^3). \quad (\text{C.6})$$

Furthermore, using the quantum decoration transformation given by eq.(40) and substituting the partial trace in eq. (C.6), we have

$$\mathbb{W}_r = \prod_{i=1}^N e^{-\beta \tilde{\mathbf{H}}_{2i-1,2i+1}} - \frac{\beta^2}{2} \sum_{j=1}^{N-1} ([\mathbf{H}'_{2j-1,2j+1}, \mathbf{H}''_{2j+1,2j+3}]) + \mathcal{O}(\beta^3), \quad (\text{C.7})$$

where we denote $\mathbf{H}'_{2j-1,2j+1} = \text{tr}_{2j}(\mathbf{H}_{2j-1,2j+1})$ and $\mathbf{H}''_{2j+1,2j+3} = \text{tr}_{2j+2}(\mathbf{H}_{2j+1,2j+3})$.

The relation below can be obtained in a similar way as obtained for (C.2). Hence, we have,

$$\begin{aligned} \prod_{i=1}^N e^{-\beta \tilde{\mathbf{H}}_{2i-1,2i+1}} &= e^{-\beta(\sum_{i=1}^N \tilde{\mathbf{H}}_{2i-1,2i+1})} \prod_{j=1}^{N-1} e^{-\beta^2 [\tilde{\mathbf{H}}_{2j-1,2j+1}, \tilde{\mathbf{H}}_{2j+1,2j+3}]}, \\ &= e^{-\beta(\sum_{i=1}^N \tilde{\mathbf{H}}_{2i-1,2i+1})} + \frac{\beta^2}{2} \sum_{j=1}^{N-1} \left([\tilde{\mathbf{H}}_{2j-1,2j+1}, \tilde{\mathbf{H}}_{2j+1,2j+3}] \right) + \mathcal{O}(\beta^3). \end{aligned} \quad (\text{C.8})$$

Finally, substituting the relation (C.8) into (C.6), the reduced operator \mathbb{W}_r is expressed by eq.(60).

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